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TITLE: WHAT IS SERIES EXTRAPOLATION ABOUT?

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ABSTRACT

The principles involved in the analytic continuation of a Taylor expansion are reviewed in the context of critical phenomena theory.

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Much of the theoretical discussion in this volume revolves around the extraction of information about the value of a function from its Taylor series expansion. For example, the problem of finding a critical index can be set out mathematically as, given the Taylor series

$$f(x) = \sum_{n=0}^{\infty} f_n x^n \tag{1}$$

find for

$$F(z) = \frac{f(z)}{f'(z)} \simeq \gamma^{-1}(z-z_0) \tag{2}$$

the physically interesting zero, z_0, of $F(z)$ and the slope, γ^{-1}, of F there. Many methods of obtaining estimates of these quantities are known and they are usually presented as formulas which relate the n^{th} estimate to the first n coefficients f_n of the Taylor expansion of $f(x)$. This mode of presentation might lead one to the hasty conclusion that series extrapolation is just a transformation of "input series data" into "output parameter estimates" without regard for intermediate aspects. The insight of the nineteenth century analysts was that the answer to this question is one of analytic continuation from information given at the point $z = 0$ to the point z_0 and is equivalent, in principle, to supplying $F(z)$ on some path from 0 to z_0. Of course, for appropriately established methods, this work has already been done for

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us. One well known example is the partial sums of the Taylor series inside its radius of convergence. However, not all methods have had the necessary work done, nor in some cases has it even been contemplated.

In order to illustrate the point, consider the example of Hardy.[1] Suppose

$$f(x) = 1 + 2x^2 + 2x^4 + 2x^6 + 2x^8 + \cdots\cdots , \tag{3}$$

which can be summed exactly for $|x| < 1$ to yield

$$f(x) = \frac{1 + x^2}{1 - x^2} . \tag{4}$$

On the other hand eq. (3) can be rearranged as

$$f(x) \stackrel{?}{=} 1 + \frac{1}{2}\left(\frac{2x}{1+x^2}\right)^2 + \frac{1}{2} \cdot \frac{3}{4}\left(\frac{2x}{1+x^2}\right)^4 + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\left(\frac{2x}{1+x^2}\right)^6 + \cdots , \tag{5}$$

which can be verified for $|x| < 1$ to be an exact rearrangement of (3) by expanding each term in (5) and comparing order-by-order in x. The new series plainly converges for small x, and indeed it gives the same answer there as do eqs. (3) and (4). However, (5) also plainly converges for very large x, which series (3) does not. For example, for x = 1000, series (5) yields 1.0000020 ····, whereas the analytic continuation of (4) yields -1.0000020 ···· which is plainly different!

What has happened? One should be careful when resumming a divergent series, e.g. series (3) for $|x| > 1$. Thus let us look at

$$1 + \frac{1}{2}\left(\frac{2x}{1+x^2}\right)^2 \lambda + \frac{1}{2} \cdot \frac{3}{4}\left(\frac{2x}{1+x^2}\right)^4 \lambda^2 + \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\left(\frac{2x}{1+x^2}\right)^6 \lambda^3 + \cdots\cdots , \tag{6}$$

which for sufficiently small λ can be summed to

$$\left[1 - \lambda\left(\frac{2x}{1+x^2}\right)^2\right]^{-1/2} = \left[\frac{1+2(1-2\lambda)x^2+x^4}{(1+x^2)^2}\right]^{-1/2} . \tag{7}$$

Now to go from $|x| < 1$ to $|x| > 1$ one must cross $|x| = 1$. If $|x| = 1$, then we may write $x = e^{i\theta}$, and

$$\frac{2x}{1+x^2} = \sec\theta \tag{8}$$

so for $|x| = 1$

$$1 < \left(\frac{2x}{1+x^2}\right)^2 < \infty \ . \tag{9}$$

For $\lambda = 1$, therefore the passage for $|x| < 1$ to $|x| > 1$ must cross the branch-cut of the square root in (7). Hence, we have the explanation of the failure of eq. (5) for $x = 1000$, in spite of the rapad convergence of the series there. There is no convergence of (5) on that point of the path from 0 to 1000 for which $|x| = 1$.

The warning of this example is that any method of series extrapolation, no matter how aesthetically appealing, must be thoroughly analyzed before it can be relied on. Padé methods[2] directly produce an approximate analytic continuation which can be cross-checked by, for example, the table of values method of Baker and Hunter.[3] For the ratio methods[3] in simple cases where

$$f(x) = A(x)\ (1 - \mu x)^{-\gamma} + B(x), \tag{10}$$

one uses the $n^{\underline{th}}$ order estimated parameters $\hat{A}_n$, $\hat{\mu}_n$ and $\hat{\gamma}_n$ to construct the orthodox, but rarely used, approximate analytic continuation

$$f_n(x) = \hat{A}_n(1-\hat{\mu}_n x)^{-\hat{\gamma}_n} + \sum_{j=0}^{n}\left[f_j - \hat{A}_n\binom{-\gamma}{j}(-\hat{\mu}_n)^j\right] x^j . \tag{11}$$

The convergence of the $f_n(x)$ can then be checked along a suitable path from $x = 0$ to $x = \hat{\mu}_n^{-1}$, and thus the convergence of the ratio method explored.

The example of Camp[4] serves well in the context of this volume as an illustration of the inadequacy of merely looking at the convergence of the "output parameter estimates." He shows how, using the first 10 terms of the very smooth looking series to some functions of the form

$$[A + Bx + (C + Dx)(1 - \mu x)^{\frac{1}{2}}](1 - \mu x)^{-5/4}, \tag{12}$$

he obtains by the "n-shifted" ratio method very good seeming convergence to a $\acute{\gamma} \simeq 1.23$ instead of the true value of 1.25. Had the corresponding $f_n(x)$ been computed and examined [here ${}_2F_1(1,\hat{\gamma}_n + \Lambda n;\ 1 + \Lambda n;\ -\hat{\mu}_n x)$ plays the role of $(1 - \hat{\mu}_n x)^{-\hat{\gamma}_n}$ in eq. (11)], a different conclusion could be foreseen. Likewise, the need for the use of orderly procedures of series analysis in the problems of actual physical interest, cannot be too strongly emphasized.

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4. W. Camp, this volume.